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Fractional Diffusion in a Solid with Mass Absorption

Yuriy Povstenko [1,*], Tamara Kyrylych [2] and Grażyna Rygał [3]

1 Institute of Mathematics and Computer Sciences, Faculty of Mathematical and Natural Sciences, Jan Długosz University in Częstochowa, al. Armii Krajowej 13/15, 42-200 Częstochowa, Poland
2 Institute of Law, Administration and Management, Faculty of Philology and History, Jan Długosz University in Częstochowa, Zbierskiego 2/4, 42-200 Częstochowa, Poland; tamara.kyrylych@gmail.com
3 Institute of Preschool and School Education, Faculty of Pedagogy, Jan Długosz University in Częstochowa, Waszyngtona 4/8, 42-200 Częstochowa, Poland; g.rygal@ajd.czest.pl
* Correspondence: j.povstenko@ajd.czest.pl; Tel.: +48-343-612-269

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Abstract: The space-time-fractional diffusion equation with the Caputo time-fractional derivative and Riesz fractional Laplacian is considered in the case of axial symmetry. Mass absorption (mass release) is described by a source term proportional to concentration. The integral transform technique is used. Different particular cases of the solution are studied. The numerical results are illustrated graphically.

Keywords: fractional calculus; Caputo derivative; Riesz derivative; Mittag-Leffler function; Laplace transform

1. Introduction

The conventional theory of diffusion is based on the classical Fick law, which relates the matter flux $\mathbf{j}$ to the concentration gradient

$$\mathbf{j} = -k\,\mathrm{grad}\,c, \tag{1}$$

where k is the diffusion conductivity.

In combination with the balance equation for mass, the classical Fick law leads to the standard diffusion equation

$$\frac{\partial c}{\partial t} = a\,\Delta c \tag{2}$$

with a being the diffusivity coefficient.

Mass transport in a medium with a first order chemical reaction is described by an additional linear source term in the diffusion equation [1]:

$$\frac{\partial c}{\partial t} = a\,\Delta c - bc, \tag{3}$$

where the values of the coefficient $b > 0$ and $b < 0$ correspond to mass absorption and mass release, respectively. Similarly, Equation (3) can also represent heat conduction with heat release or absorption [2]. This equation also governs heat transfer in a thin plate whose lateral surfaces exchange heat with the ambient medium having constant temperature; the values $b > 0$ and $b < 0$ correspond to the temperature of the medium greater and less than that of the plate, respectively [3]. Similar equations appear in the theory of bio-heat transfer [4–6] and in the survival probability (see [7] and references therein).

Nonclassical theories, in which the Fick law and the standard diffusion equation are replaced by more general equations, constantly attract the attention of researchers. From a mathematical point of view, the Fick law in the theory of diffusion, the Fourier law in the theory of heat conduction, and the Darcy law in the theory of fluid flow through a porous medium are identical. Some of the generalized theories are formulated in terms of diffusion, others in terms of heat conduction or fluid flow through a porous medium.

The time-nonlocal dependence between the matter flux $\mathbf{j}$ and the concentration gradient grad c with the long-tail power kernel (see [8–11]) can be interpreted in terms of fractional integrals and derivatives and results in the time-fractional diffusion equation

$$\frac{\partial^\alpha c}{\partial t^\alpha} = a\,\Delta\, c\,, \tag{4}$$

where $\partial^\alpha c\,/\partial t^\alpha$ is the Caputo fractional derivative [12–14]:

$$\frac{\partial^\alpha f(t)}{\partial t^\alpha} = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} \frac{\mathrm{d}^n f(\tau)}{\mathrm{d}\tau^n}\, \mathrm{d}\tau, \qquad n-1<\alpha<n, \tag{5}$$

and $\Gamma(\alpha)$ is the gamma function.

The Caputo fractional derivative has the following Laplace transform rule

$$\mathcal{L}\left\{\frac{\partial^\alpha f}{\partial t^\alpha}\right\} = s^\alpha f^*(s) - \sum_{k=0}^{n-1} f^{(k)}(0^+) s^{\alpha-1-k}, \qquad n-1<\alpha<n. \tag{6}$$

Here the asterisk denotes the transform, s is the Laplace transform variable.

Space nonlocal generalizations of the Fick law with the power kernel can also be interpreted in terms of fractional calculus and give the space-fractional diffusion equation

$$\frac{\partial c}{\partial t} = -a\,(-\Delta)^{\beta/2}\, c\,, \tag{7}$$

where the positive powers of the Laplace operator $-(-\Delta)^{\beta/2}$, $\beta>0$, are called the Riesz derivatives.

The space-fractional heat conduction equation in the case of one spatial coordinate was considered by Gorenflo and Mainardi [15], in the case of higher dimensions by Hanyga [16]. The definitions of space-fractional differential operators can be found, for example, in [14,17–20].

The cumbersome aspects of space-fractional differential operators disappear when one computes their Fourier transforms:

$$\mathcal{F}\left\{(-\Delta)^{\beta/2} f(\mathbf{x})\right\} = |\boldsymbol{\xi}|^\beta \mathcal{F}\left\{f(\mathbf{x})\right\}, \qquad \beta>0, \tag{8}$$

where $\boldsymbol{\xi}$ is the transform-variable vector.

It is obvious that Equation (8) is a fractional generalization of the standard formula for the Fourier transform of the Laplace operator corresponding to $\beta=2$:

$$\mathcal{F}\Big\{\,(-\Delta)\, f(\mathbf{x})\Big\} = |\boldsymbol{\xi}|^2 \mathcal{F}\Big\{f(\mathbf{x})\Big\}. \tag{9}$$

If the considered function $f(x,y)$ depends only on the radial coordinate $r=\left(x^2+y^2\right)^{1/2}$, then the two-fold Fourier transform

$$\widetilde{f}(\xi,\eta) = \frac{1}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y)\, \mathrm{e}^{i(x\xi+y\eta)}\mathrm{d}x\,\mathrm{d}y \tag{10}$$

can be simplified (see [11,21]) and is expressed as

$$\begin{aligned}\mathcal{F}\Big\{f(x,y)\Big\} &= \widetilde{f}(\xi,\eta) = \mathcal{H}\Big\{f(r)\Big\} \\ &= \widehat{f}(\varrho) = \int\limits_0^\infty r f(r)\, J_0(r\varrho)\,\mathrm{d}r,\end{aligned} \tag{11}$$

$$\begin{aligned}\mathcal{F}^{-1}\left\{\widetilde{f}(\xi,\eta)\right\} &= f(x,y) = \mathcal{H}^{-1}\left\{\widehat{f}(\varrho)\right\} \\ &= f(r) = \int\limits_0^\infty \varrho \widehat{f}(\rho)\, J_0(r\varrho)\,\mathrm{d}\varrho\,,\end{aligned} \tag{12}$$

where $\varrho = |\boldsymbol{\xi}| = \sqrt{\xi^2+\eta^2}$. Hence, in the case of axial symmetry the two-fold Fourier transform with respect to the Cartesian coordinates x and y is reduced to the Hankel transform with respect to the radial coordinate r. Here $J_0(r)$ is the Bessel function of the first kind of the zeroth order, the tilde marks the Fourier transform, the hat denotes the Hankel transform.

Equation (8) for the Fourier transform of the fractional Laplace operator in the case of axial symmetry also simplifies:

$$\mathcal{F}\left\{(-\Delta)^{\beta/2} f(x,y)\right\} = \mathcal{H}\left\{(-\Delta)^{\beta/2} f(r)\right\} = \varrho^{\beta}\widehat{f}(\varrho). \tag{13}$$

If the time nonlocality is accompanied with the spatial nonlocalty, then the general space-time-fractional heat conduction equation is obtained (see [18,19,22,23]):

$$\frac{\partial^\alpha c}{\partial t^\alpha} = -a\,(-\Delta)^{\beta/2}\,c\,. \tag{14}$$

It should be emphasized that fractional calculus (the theory of derivatives and integrals of non-integer order) has many important applications in description of processes in media with complex internal structure: in fractional dynamics [24–27], fractional kinetics [28–30], fractional thermoelasticity [8,9,31,32], biology [33,34], fractional control [35–37], description of physical processes in colloid, glassy and porous materials [38–40], comb structures [41,42], dielectrics and semiconductors [30,43,44], among others.

The fractional counterpart of Equation (3) has the following form:

$$\frac{\partial^\alpha c}{\partial t^\alpha} = -a\,(-\Delta)^{\beta/2}\,c - bc. \tag{15}$$

Physical aspects of fractional reaction-diffusion were extensively studied in the literature (see, for example, [45–49] and references therein).

In this paper, we study the fundamental solutions to the Cauchy problem and to the source problem for Equation (15) in the case of axial symmetry. The integral transform technique is used. The numerical results are illustrated graphically.

2. Fundamental Solution to the Cauchy Problem

We consider the space-time-fractional diffusion equation with mass absorption (mass release) in the axisymmetric case:

$$\frac{\partial^\alpha c}{\partial t^\alpha} = -a\,(-\Delta)^{\beta/2}\,c - bc, \quad 0<\alpha\le 1, \quad 1\le\beta\le 2, \tag{16}$$

under the initial condition

$$t=0:\quad c = \frac{p_0}{2\pi r}\,\delta(r-R), \tag{17}$$

where $\delta(r)$ is the Dirac delta function.

The constant multiplier p_0 has been introduced in Equation (17) to get the nondimensional quantities used in numerical calculations (see Equation (30)).

The Laplace transform with respect to time t and the Hankel transform with respect to the radial coordinate r give the solution in the transform domain

$$\widehat{c}^{*} = \frac{p_0}{2\pi} \frac{s^{\alpha-1}}{s^{\alpha} + a\varrho^{\beta} + b} J_0\left(R\varrho\right). \tag{18}$$

After inversion of the integral transforms, we get:

$$c(r,t) = \frac{p_0}{2\pi} \int\limits_0^{\infty} E_{\alpha}\left[-\left(a\varrho^{\beta} + b\right) t^{\alpha}\right] J_0\left(R\varrho\right) J_0\left(r\varrho\right) \varrho \, \mathrm{d}\varrho, \tag{19}$$

where $E_{\alpha}(z)$ is the Mittag-Leffler function in one parameter α [12,14,50]:

$$E_{\alpha}\left(z\right) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \quad \alpha > 0, \quad z \in C, \tag{20}$$

and the following formula for the inverse Laplace transform

$$\mathcal{L}^{-1}\left\{\frac{s^{\alpha-1}}{s^{\alpha} + b}\right\} = E_{\alpha}\left(-bt^{\alpha}\right) \tag{21}$$

has been used.

The asymptotic behavior of the solution is determined by the asymptotic behavior of the Mittag-Leffler function $E_{\alpha}(-x)$. For $0 < \alpha < 1$, we have [51–53] :

$$E_{\alpha}\left[-\left(a\varrho^{\beta} + b\right) t^{\alpha}\right] \sim \exp\left[-\frac{\left(a\varrho^{\beta} + b\right) t^{\alpha}}{\Gamma(1+\alpha)}\right] \quad \text{for small values of } t\,, \tag{22}$$

$$E_{\alpha}\left[-\left(a\varrho^{\beta} + b\right) t^{\alpha}\right] \sim \frac{1}{\Gamma(1-\alpha)} \frac{1}{\left(a\varrho^{\beta} + b\right) t^{\alpha}} \quad \text{for large values of } t\,. \tag{23}$$

Consider several particular cases of the obtained solution corresponding to different particular cases of the Mittag-Leffler function.

2.1. Standard Diffusion ($\alpha = 1$, $\beta = 2$)

Since $E_1(-x) = \mathrm{e}^{-x}$, taking into account integral (A1) from Appendix A, we get

$$c(r,t) = \frac{p_0}{4\pi a t} I_0\left(\frac{rR}{2at}\right) \exp\left(-\frac{r^2 + R^2}{4at} - bt\right). \tag{24}$$

2.2. Localized Diffusion ($\alpha \to 0$, $\beta = 2$)

In this case $E_0(-x) = \frac{1}{1+x^2}$ and using Equation (A2), we obtain

$$c(r,t) = \frac{p_0}{2\pi a} \begin{cases} I_0\left[\dfrac{r(1+b)}{\sqrt{a}}\right] K_0\left[\dfrac{R(1+b)}{\sqrt{a}}\right], & 0 \le r \le R, \\[2ex] I_0\left[\dfrac{R(1+b)}{\sqrt{a}}\right] K_0\left[\dfrac{r(1+b)}{\sqrt{a}}\right], & R \le r < \infty. \end{cases} \tag{25}$$

2.3. Subdiffusion with $\alpha = 1/2$ and $\beta = 2$

The Mittag-Leffler function $E_{1/2}(-x)$ can be written in the following integral form [11]:

$$E_{1/2}(-x) = \frac{2}{\sqrt{\pi}} \int_0^\infty \exp\left(-u^2 - 2ux\right) \mathrm{d}u. \tag{26}$$

From Equations (19) and (26) with taking into account (A1), we have

$$\begin{aligned} c(r,t) &= \frac{p_0}{4\pi^{3/2} a t^{1/2}} \int_0^\infty I_0\left(\frac{rR}{4at^{1/2}u}\right) \\ &\times \exp\left(-u^2 - 2bt^{1/2}u - \frac{r^2+R^2}{8at^{1/2}u}\right) \frac{1}{u}\, \mathrm{d}u. \end{aligned} \tag{27}$$

2.4. Cauchy Diffusion with $\alpha = 1$, $\beta = 1$

For the so called Cauchy diffusion [22], which is characterized by the values $\alpha = \beta = 1$, evaluating the corresponding integral (see Equation (A3) from Appendix A), we arrive at

$$c(r,t) = \frac{p_0 a t}{8\pi^2} \mathrm{e}^{-bt} \frac{k^3 \mathbf{E}(k)}{(1-k^2)(rR)^{3/2}}, \tag{28}$$

where $\mathbf{E}(k)$ is the complete elliptic integral of the first kind,

$$k = \frac{2\sqrt{rR}}{\sqrt{(at)^2 + (r+R)^2}}. \tag{29}$$

Results of numerical calculations are shown in Figures 1–4. We have introduced the following nondimensional quantities

$$\bar{c} = \frac{2\pi R^2}{p_0} c, \quad \bar{r} = \frac{r}{R}, \quad \bar{t} = \sqrt{\frac{a t^\alpha}{R^\beta}}, \quad \bar{b} = t^\alpha b. \tag{30}$$

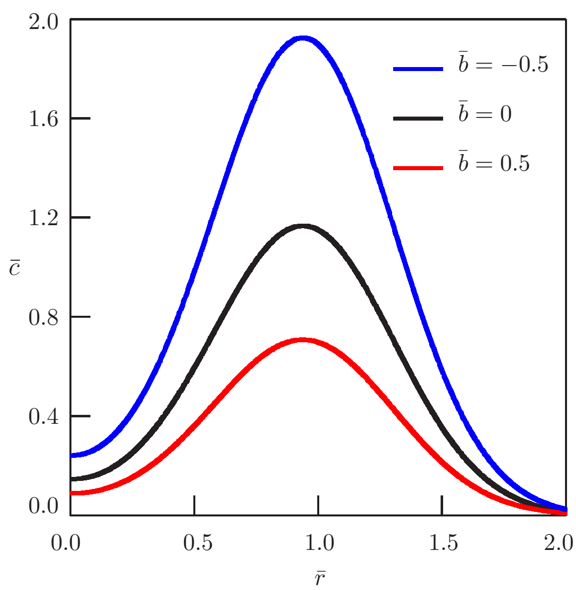

Figure 1. Dependence of the fundamental solution to the Cauchy problem on distance for $\alpha = 1$, $\beta = 2$, $\bar{t} = 0.25$ and various values of $\bar{b}$.

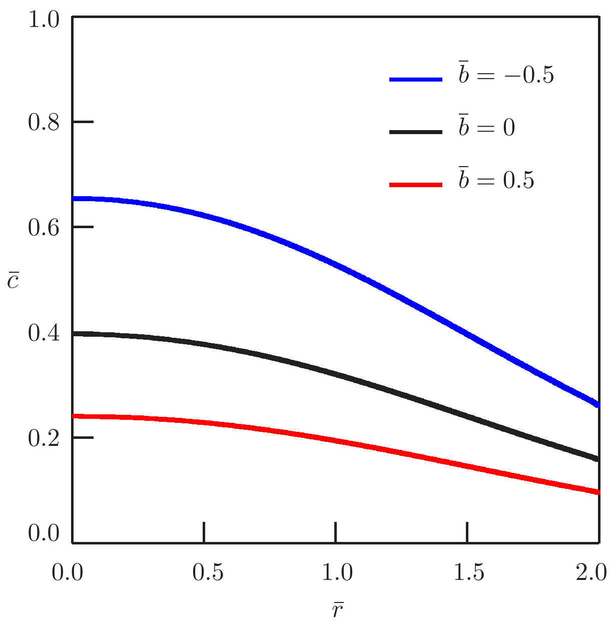

Figure 2. Dependence of the fundamental solution to the Cauchy problem on distance for $\alpha = 1$, $\beta = 2$, $\bar{t} = 1$ and various values of $\bar{b}$.

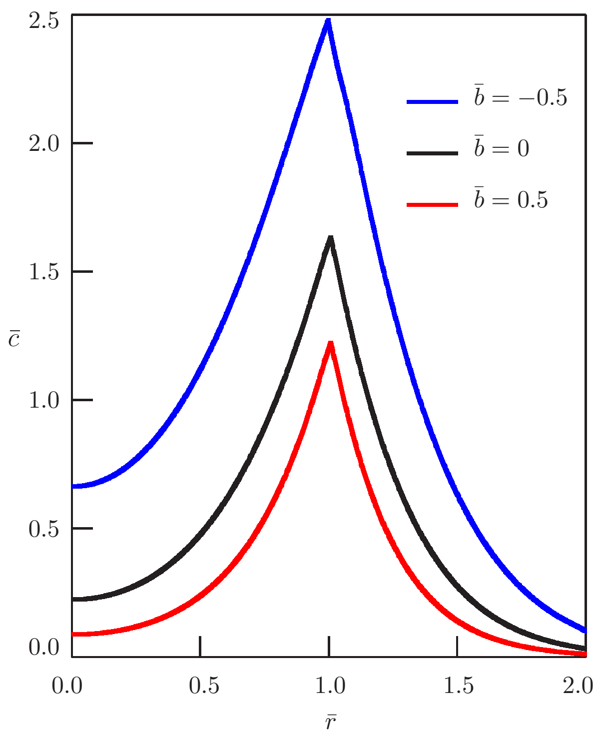

Figure 3. Dependence of the fundamental solution to the Cauchy problem on distance for $\alpha = 0.5$, $\beta = 2$, $\bar{t} = 0.25$ and various values of $\bar{b}$.

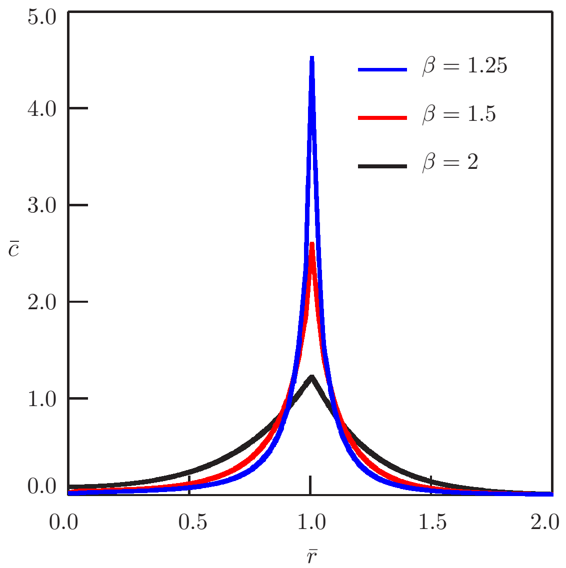

Figure 4. Dependence of the fundamental solution to the Cauchy problem on distance for $\alpha = 0.5$, $\bar{t} = 0.25$, $\bar{b} = 0.5$ and various values of β.

3. Fundamental Solution to the Source Problem

In this case, we study the equation

$$\frac{\partial^\alpha c}{\partial t^\alpha} = -a\left(-\Delta\right)^{\beta/2} c - bc + \frac{q_0}{2\pi r}\,\delta(t)\,\delta(r-R), \qquad 0<\alpha\le 1, \quad 1\le\beta\le 2, \tag{31}$$

under zero initial condition

$$t=0: \quad c=0. \tag{32}$$

The Laplace transform with respect to time t and the Hankel transform with respect to the radial coordinate r give the solution in the transform domain

$$\hat{c}^* = \frac{q_0}{2\pi}\,\frac{1}{s^\alpha + a\varrho^\beta + b}\,J_0\left(R\varrho\right). \tag{33}$$

After inversion of the integral transforms, we arrive at

$$c(r,t) = \frac{q_0 t^{\alpha-1}}{2\pi}\int\limits_0^\infty E_{\alpha,\alpha}\left[-\left(a\varrho^\beta + b\right)t^\alpha\right] J_0\left(R\varrho\right) J_0\left(r\varrho\right)\varrho\,\mathrm{d}\varrho, \tag{34}$$

where $E_{\alpha,\gamma}(z)$ is the Mittag-Leffler function in two parameters α and γ [12,14,50]:

$$E_{\alpha,\gamma}\left(z\right) = \sum_{n=0}^\infty \frac{z^n}{\Gamma(\alpha n+\gamma)}, \quad \alpha>0, \quad \gamma>0, \quad z\in C, \tag{35}$$

and

$$\mathcal{L}^{-1}\left\{\frac{s^{\alpha-\gamma}}{s^\alpha+b}\right\} = t^{\gamma-1}E_{\alpha,\gamma}\left(-bt^\alpha\right). \tag{36}$$

Subdiffusion with $\alpha = 1/2$ *and* $\beta = 2$

The Mittag-Leffler function $E_{1/2,1/2}(-x)$ is presented as [11]:

$$E_{1/2,1/2}(-x) = \frac{2}{\sqrt{\pi}} \int_0^\infty \exp\left(-u^2 - 2ux\right) u \, du. \tag{37}$$

Hence

$$\begin{aligned} c(r,t) &= \frac{p_0}{4\pi^{3/2} a t^{1/2}} \int_0^\infty I_0\left(\frac{rR}{4at^{1/2}u}\right) \\ &\times \exp\left(-u^2 - 2bt^{1/2}u - \frac{r^2+R^2}{8at^{1/2}u}\right) du. \end{aligned} \tag{38}$$

The results of numerical calculations are shown in Figures 5 and 6, where the nondimensional concentration is defined as

$$\bar{c} = \frac{2\pi R^2}{q_0 t^{\alpha-1}} c, \tag{39}$$

other nondimensional quantities are the same as in (30).

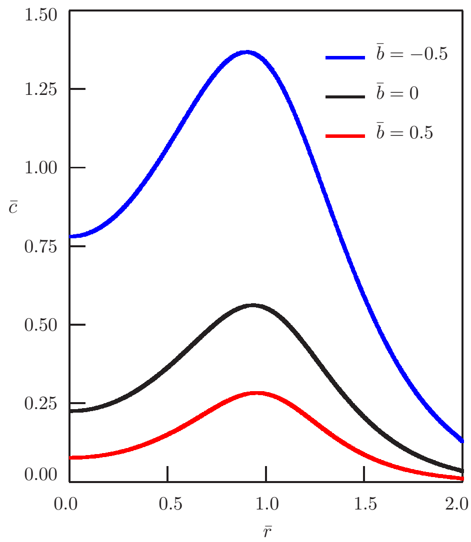

Figure 5. Dependence of the fundamental solution to the source problem on distance for $\alpha = 0.5$, $\beta = 2$, $\bar{t} = 0.25$ and various values of $\bar{b}$.

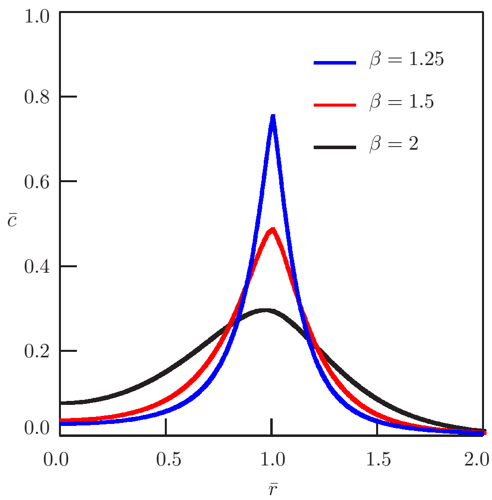

Figure 6. Dependence of the fundamental solution to the source problem on distance for $\alpha = 0.5$, $\bar{t} = 0.25$, $\bar{b} = 0.5$ and various values of β.

4. Discussion

We have considered the fundamental solutions to the Cauchy problem and to the source problem for the space-time fractional diffusion equation with the linear source term. Time nonlocality deals with memory effects, whereas space nonlocality describes the long-range interaction. It is seen from Figures that for positive values of the parameter b (mass absorption) the mass concentration is decreased, for negative values of the parameter b (mass release) the mass concentration is increased. For $\alpha = 1$, the shape of curves depends on the value of nondimensional time $\bar{t}$ (Figure 1 presents typical results for small values of $\bar{t}$, Figure 2—for $\bar{t} \geq 1$). For fractional value of α, the fundamental solution to the Cauchy problem has a cusp at $\bar{r} = 1$. Such a cusp also appears in the curves describing the fundamental solution to the source problem for decreasing value of the order of fractional Laplacian (compare Figures 4 and 6). To calculate the Mittag-Leffler functions $E_\alpha(z)$ in the fundamental solution (19) and $E_{\alpha,\beta}(z)$ in the fundamental solution (34) we have used the algorithms proposed in [54].

Author Contributions: Yuriy Povstenko and Tamara Kyrylych wrote the paper; Grażyna Rygał carried out numerical calculations for the fundamental solution to the source problem and prepared the corresponding Figures; Tamara Kyrylych performed numerical calculations for the Cauchy problem and prepared the corresponding Figures. All the authors have equally contributed in the discussion and overall preparation of the manuscript, as well as read and improved the final version of the manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Integrals

In Appendix, we present integrals used in the paper. Equations (A1) and (A2) are taken from [55], the Lipshitz-Hankel integral (A3) was evaluated in [56].

$$\int_0^\infty \mathrm{e}^{-ax^2} J_0(bx)\, J_0(cx)\, x\, \mathrm{d}x = \frac{1}{2a} \exp\left(-\frac{b^2+c^2}{4a}\right) I_0\left(\frac{bc}{2a}\right), \qquad a>0, \quad b>0, \quad c>0. \tag{A1}$$

$$\int_0^\infty \frac{x}{x^2+a^2} J_0(bx)\, J_0(cx)\, \mathrm{d}x = \begin{cases} I_0(ab)\, K_0(ac), & 0<b<c, \\ I_0(ac)\, K_0(bc), & 0<c<b, \end{cases} \qquad a>0. \tag{A2}$$

$$\int_0^\infty \mathrm{e}^{-ax} J_0(bx)\, J_0(cx)\, x\, \mathrm{d}x = \frac{ak^3}{4\pi(1-k^2)(bc)^{3/2}} \mathbf{E}(k), \qquad a>0, \ b>0, \ c>0, \tag{A3}$$

where $\mathbf{E}(k)$ is is the complete elliptic integral of the first kind,

$$k = \frac{2\sqrt{bc}}{\sqrt{a^2+(b+c)^2}}.$$

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